1,10-Phenanthroline

66-71-7 | DTXSID1025857

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 7.38

Global applicability domain: Inside

Local applicability domain index: 9.98e-01

Confidence level: 8.24e-01

Nearest Neighbors from the Training Set

Image not found
4,4'-Dichlorobiphenyl
Measured: 7.68
Predicted: 7.38

Image not found
2,2'-Dichlorobiphenyl
Measured: 7.18
Predicted: 7.38

Image not found
2,4'-Dichlorobiphenyl
Measured: 7.40
Predicted: 7.38

Image not found
1,3,5-Trichloronaphthalene
Measured: 7.32
Predicted: 7.45